Trimethyl phosphate 512-56-1 | DTXSID1021403

Model Performance

| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (7 | 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|--------------|-----------------|------|----------------|------|------------|--|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE | |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 | |

Model Results

Predicted value: -49.9 °C

Global applicability domain: Inside

Local applicability domain index: 6.39e-01

Confidence level: 6.91e-01

Nearest Neighbors from the Training Set

Image not found

Trimethyl phosphate
Measured: -46.0
Predicted: -49.9

Image not found

Triethyl phosphate Measured: -56.4 Predicted: -54.1

Image not found

Dimethyl hydrogen phosphite

Measured: -60 0

Measured: -60.0 Predicted: -61.6

Image not found

Diisopropyl fluorophosphate

Measured: -82.0 Predicted: -73.2